

Amendment to the Claims:

This listing of claims will replace all prior versions, and listing, of claims in the application.

Listing of Claims:

1. (currently amended) A computer implemented method of ~~selecting~~ a generating representative three dimensional ~~conformation~~ conformations of reactant molecules comprising the steps of:
 - a) defining a set of topomeric alignment rules; and
 - b) applying the topomeric alignment rules to the reactants to generate the representative conformations.
2. (new) A computer implemented method of generating representative three dimensional conformations of fragments comprising the steps of:
 - a) defining a set of topomeric alignment rules; and
 - b) applying the topomeric alignment rules to the fragments to generate the representative conformations.
3. (new) A computer implemented method of characterizing the three dimensional structure of reactants, which can assume many conformations, comprising the steps of:
 - a) generating representative three dimensional conformations of reactant molecules comprising the steps of:
 - (1) defining a set of topomeric alignment rules; and
 - (2) applying the topomeric alignment rules to the reactants to generate the

representative conformations; and

- b) determining the CoMFA steric fields for each aligned reactant.
4. (new) The method of claim 3 further comprising the addition of topomeric hydrogen bonding fields to the CoMFA steric fields.
5. (new) A computer implemented method of characterizing the three dimensional structure of fragments, which can assume many conformations, comprising the steps of:
- a) generating representative three dimensional conformations of fragments comprising the steps of:
 - (1) defining a set of topomeric alignment rules; and
 - (2) applying the topomeric alignment rules to the fragments to generate the representative conformations; and
 - b) determining the CoMFA steric fields for each aligned fragment.
6. (new) The method of claim 5 further comprising the addition of topomeric hydrogen bonding fields to the CoMFA steric fields.
7. (new) A computer implemented method of applying a molecular structural descriptor to a set of reactants comprising the following steps:
- a) generating representative three dimensional conformations of reactant molecules comprising the steps of:
 - (1) defining a set of topomeric alignment rules; and
 - (2) applying the topomeric alignment rules to the reactants to generate the representative conformations; and

- b) determining the CoMFA steric fields for each topomerically aligned reactant; and
 - c) calculating the field differences between all pairs of reactants.
8. (new) The method of claim 7 further comprising after step b the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.
9. (new) A computer implemented method of applying a molecular structural descriptor to a set of fragments comprising the following steps:
- a) generating representative three dimensional conformations of fragments comprising the steps of:
 - (1) defining a set of topomeric alignment rules; and
 - (2) applying the topomeric alignment rules to the fragments to generate the representative conformations; and
 - b) determining the CoMFA steric fields for each topomerically aligned fragment; and
 - c) calculating the field differences between all pairs of fragments.
10. (new) The method of claim 9 further comprising after step b the additional step of adding topomeric hydrogen bonding fields to the CoMFA fields.